GOALI/FRG: Structural Properties of Alumina and Adsorbed Metal Particles

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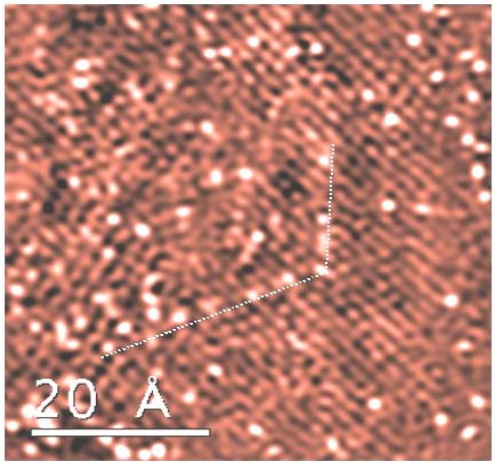
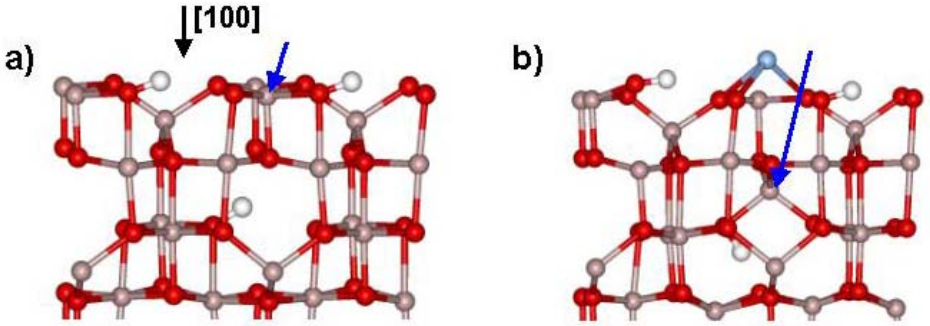
Some transition alumina (Al_2O_3) polytypes are widely used as a catalytic support (on which catalyst metal particles are dispersed). However, at temperatures in the range 1000-1200ºC, they transform rapidly into the thermodynamically stable α-alumina phase, and the catalytic activity stops. We combined theoretical and experimental tools to obtain a comprehensive microscopic account of the transformation process and of the role of dopants, such as La, to impede it. The stabilization is a result of interaction between a dopant and the alumina surface that may cause a significant surface relaxation. Another objective has been to investigate the structure and catalytic behavior of metal particles (Cr, Rh, Pd, Pt, etc.) on the alumina surfaces.

Physical Review B **67**, 115414 (2003);

Nature (submitted).



Z-contrast image of a sample of La-doped γ-Al_2O_3. Bright spots correspond to La atoms.



Schematics of the configurations for the (100) surface of γ-Al_2O_3, determined by first-principles calculations: (a) undoped, and (b) La-doped. When the La atoms is present on the surface, a surface Al atom relaxes from the surface into a cation vacancy.

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Education, training, and development:
Two undergraduates (John Ash and Ari B. Silver), one graduate student (Ying Hu), and two postdocs (Albina Borisevich and Shuhui Cai) contributed to this work. Prof. Karl Sohlberg (co-PI) got a prestigious "DuPont Young Professor" award for his work on computational materials science (including his work on transition aluminas and their phase transformations). The universities benefited from visits of the industrial collaborators and their presentations for the materials science/material physics community. A very productive collaboration with scientists from the Russian Academy of Sciences has been established.

Other specific products:
This project has stimulated the upgrade of the existing scanning transmission electron microscopy (STEM) facility at Oak Ridge National Laboratory. At present, the STEM has the world's highest resolution for Z-contrast imaging and after upgrading (to be finally completed in the fall of 2003) this resolution will be enhanced to about 0.5 Å for both Z-contrast imaging and EELS. The smaller beam size provides greatly improved signal to noise ratio for single atoms and crystals, and will greatly facilitate the direct imaging of dopant and impurity sites both on the alumina surface and in the bulk. A new facility, the Advanced Materials Characterization Facility is due to be constructed within a year to house these upgraded instruments.